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ROSENBROCK TIME INTEGRATION FOR UNSTEADY FLOW SIMULATIONS

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Abstract. This contribution compares the efficiency of Rosenbrock time integration schemes with ESDIRK schemes, applicable to unsteady flow and fluid-structure interaction simulations. Compared to non-linear ESDIRK schemes, the linear implicit Rosenbrock-Wanner schemes require subsequent solution of the same linear systems with different right hand sides. By solving the linear systems with the iterative solver GMRES, the preconditioner can be reused for the subsequent stages of the Rosenbrock-Wanner scheme. Unsteady flow simulations show a gain in computational efficiency of approximately factor three to five in comparison with ESDIRK.

1 INTRODUCTION

Efficient time integration methods applicable to fluid dynamics and fluid-structure interaction simulations are of high importance. High order time integration methods are employed in order to increase the efficiency of unsteady computations. Currently, second order implicit schemes are commonly used in engineering codes [1]. The use of implicit methods is advised, since explicit methods impose strict stability constraints on the time step used by the method. Contrary to explicit methods, the time step for implicit methods can be chosen based on accuracy considerations. For fluid flows, large differences in length and time scales are present, namely in the boundary layer, which increase the stiffness of the system. Therefore, implicit schemes are preferred over explicit schemes for fluid solvers.

This contribution compares the computational efficiency and accuracy of implicit Runge-Kutta schemes, namely ESDIRK, with Rosenbrock-Wanner schemes for a non-linear convection-diffusion problem and a two-dimensional laminar flow problem [2]. Rosenbrock-Wanner methods follow from a linearisation of a DIRK scheme, thereby loosing some stability and accuracy properties of the implicit Runge-Kutta scheme, but the computational costs per time step are reduced. As a result of the linearisation step, the linear implicit Rosenbrock-Wanner scheme consists of solving the subsequent stages with constant system matrix and varying right hand sides. The preconditioner can be reused for all the stages of the scheme.

The paper is structured as follows. ESDIRK and Rosenbrock-Wanner time integration schemes are discussed in Section 2. The Newton-Krylov method is shortly discussed in Section 3. The results for a non-linear convection-diffusion problem and for a uniform flow around a cylinder are shown in Section 4 and 5, respectively. Section 6 finalises this paper with the conclusions.

2 TIME INTEGRATION SCHEMES

The method of lines paradigm is followed in this paper. Therefore, the non-linear convection-diffusion problem, and the Navier-Stokes equations are discretised in space and in time. The initial value problem of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{w}(\mathbf{t}) = \mathbf{F}(\mathbf{w}(t)), \qquad \mathbf{w}(0) = \mathbf{w}^0 \tag{1}$$

is solved for a known initial solution $\mathbf{w}^0$, where $\mathbf{F}$ represents the spatial discretisation of the convection-diffusion problem or Navier-Stokes equations. ESDIRK and Rosenbrock-Wanner time integration schemes are considered for this study, and discussed in Section 2.1 and 2.2. The used adaptive time step control method is shortly laid out in Section 2.3.

2.1 ESDIRK schemes

Explicit first stage, single diagonal, diagonally implicit Runge-Kutta (ESDIRK) methods are a subclass of SDIRK methods, and as a consequence are L-stable for any design order. The ESDIRK method is given by

$$\mathbf{w}^{(i)} = \mathbf{w}^n + \Delta t \sum_{j=1}^{s} a_{ij}\, \mathbf{F}^{(j)}, \qquad \mathbf{F}^{(j)} = \mathbf{F}\left(\mathbf{w}^{(j)}\right), \qquad i = 1, ..., s \tag{2}$$

wherein $\mathbf{w}^{(i)}$ are the stage values, and Δt is the used time step. The solution at the next time level $\mathbf{w}^{n+1}$ is computed with

$$\mathbf{w}^{n+1} = \mathbf{w}^n + \Delta t \sum_{j=1}^{s} b_j\, \mathbf{F}^{(j)}. \tag{3}$$

A lower order solution $\widehat{\mathbf{w}}^{n+1}$ can be determined with

$$\widehat{\mathbf{w}}^{n+1} = \mathbf{w}^n + \Delta t \sum_{j=1}^{s} \widehat{b}_j \, \mathbf{F}^{(j)}, \tag{4}$$

which is used by the adaptive time step control algorithm to efficiently calculate an error estimate for the time step. The coefficients a_{ij}, b_j and $\widehat{b}_j$ can be found in a Butcher tableau. The coefficients of the used schemes are shown in [3, 4].

The first stage of an ESDIRK method is explicit, i.e. $a_{11} = 0$. Hence, $s - 1$ non-linear systems need to be solved. Also, the solution at the last stage of the method is equal to the solution at the next time step, thus $a_{sj} = b_j$. The implicit stages can be solved with a multi grid method or a Newton-Krylov method.

2.2 Rosenbrock-Wanner schemes

Rosenbrock, Rosenbrock-Wanner or ROW-schemes are part of a class of linearly implicit Runge-Kutta methods. Rosenbrock methods replace non-linear systems with a sequence of linear systems, and are derived by linearizing a DIRK scheme. As a result, some stability and accuracy properties are lost, but the computational costs per time step are reduced: s linear equation systems with a constant coefficient matrix and different right hand sides need to be solved, instead of s non-linear systems.

An s-stage Rosenbrock method is described with the following relation:

$$(\mathbf{I} - \Delta t \, \gamma_{ii} \, \mathbf{J}) \, \mathbf{w}^{(i)} = \Delta t \, \mathbf{F} \left(\mathbf{w}^n + \sum_{j=1}^{i-1} \alpha_{ij} \, \mathbf{w}^{(j)} \right) + \Delta t \, \mathbf{J} \sum_{j=1}^{i-1} \gamma_{ij} \, \mathbf{w}^{(j)}, \qquad i = 1, ..., s. \tag{5}$$

The solution at the next time step $\mathbf{w}^{n+1}$ is determined with

$$\mathbf{w}^{n+1} = \mathbf{w}^n + \sum_{j=1}^{s} b_j \, \mathbf{w}^{(j)}. \tag{6}$$

A lower order estimation $\widehat{\mathbf{w}}^{n+1}$ can be found by evaluating

$$\widehat{\mathbf{w}}^{n+1} = \widehat{\mathbf{w}}^n + \sum_{j=1}^{s} \widehat{b}_j \, \mathbf{w}^{(j)}. \tag{7}$$

The coefficients α_{ij}, γ_{ij} and b_j are generally shown in a Butcher tableau.

In order to accelerate the computations, the Jacobians $\mathbf{J}\left(\mathbf{w}^{(i)}\right)$ are replaced by $\mathbf{J} = \mathbf{J}\left(\mathbf{w}_n\right)$, such that the Jacobian needs to be evaluated only once during the Rosenbrock computation [5]. W-methods are obtained, if an approximation for the Jacobian is used. W-methods have additional order conditions. Krylov-ROW schemes are applied, if a Krylov subspace method is used to compute a solution for the linear system.

For implementation purposes, Equations (5) and (6) can be rewritten by introducing the new variables $\mathbf{u}^{(i)}$. This approach is applied, since a direct implementation of Equations (5) and (6) requires the solution of a linear system with the matrix $\mathbf{I} - \Delta t\, \gamma_{ii}\, \mathbf{J}$ and the matrix-vector multiplication $\mathbf{J} \cdot \sum \gamma_{ij}\, \mathbf{w}^{(j)}$. This matrix-vector multiplication is avoided by introducing the new variables $\mathbf{u}^{(i)}$:

$$\mathbf{u}^{(i)} = \sum_{j=1}^{i} \gamma_{ij}\, \mathbf{w}^{(j)} \qquad i = 1, ..., s. \tag{8}$$

If $\gamma_{ij} \neq 0$ for $j \leqslant i$, then the matrix $\mathbf{\Gamma} = (\gamma_{ij})$ is invertible and $\mathbf{w}^{(i)}$ can be determined from $\mathbf{u}^{(i)}$ with

$$\mathbf{w}^{(i)} = \frac{1}{\gamma_{ii}}\, \mathbf{u}^{(i)} - \sum_{j=1}^{i-1} c_{ij}\, \mathbf{u}^{(j)}, \tag{9}$$

wherein $\mathbf{C}$ is given by $\mathbf{C} = \mathrm{diag}\,({\gamma_{11}}^{-1}, ..., {\gamma_{ss}}^{-1}) - \mathbf{\Gamma}^{-1}$.

Thus the following formulation of the Rosenbrock method is found for practical implementations,

$$\mathbf{L}\, \mathbf{u}^{(i)} = \mathbf{F} \left(\mathbf{w}^n + \sum_{j=1}^{i-1} a_{ij} \mathbf{u}^{(j)} \right) + \frac{1}{\Delta t} \sum_{j=1}^{i-1} c_{ij} \mathbf{u}^{(j)}, \qquad i = 1, ..., s, \tag{10}$$

with $\mathbf{L} = \left(\dfrac{1}{\Delta t\, \gamma} \mathbf{I} - \mathbf{J} \right)$, and $\gamma = \gamma_{ii}$, thus $\mathbf{L}$ is constant for the consecutive stages of the Rosenbrock scheme. The solution at the next time step $\mathbf{w}^{n+1}$ is given by

$$\mathbf{w}^{n+1} = \mathbf{w}^n + \sum_{j=1}^{s} m_j\, \mathbf{u}^{(j)}, \tag{11}$$

wherein the coefficients a_{ij} and m_j are given by $(a_{ij}) = (\alpha_{ij})\, \mathbf{\Gamma}^{-1}$ and $(m_1, ..., m_s) = (b_1, ..., b_s)\, \mathbf{\Gamma}^{-1}$. The coefficients of the used ROW-schemes can be found in [6, 7, 8, 9].

Concluding, Rosenbrock-type methods are presented as an alternative to ESDIRK time integration schemes. Rosenbrock-Wanner methods can be used, which use an approximation for the Jacobian, thus effectively reducing the computational costs per time step. However, the accuracy and stability are also reduced per time step. When Krylov-ROW schemes are applied, a Krylov subspace method is used to compute the solution for the linear system resulting from the Rosenbrock scheme.

2.3 Adaptive time step control

Time step control is an important measure to increase the efficiency and robustness of a time integration method. A constant time step often results in a large number of small steps, increasing the computational costs of a simulation significantly.

For Runge-Kutta and Rosenbrock schemes, an embedded scheme can be used as an error estimator:

$$r^n = ||\widehat{\mathbf{w}}^{n+1} - \mathbf{w}^n||. \tag{12}$$

A digital filter is used for the selection of the time step, as discussed in [10]. The next time step is computed with

$$\Delta t^{n+1} = \left(\frac{\epsilon}{r^n}\right)^{\beta_1} \left(\frac{\epsilon}{r^{n-1}}\right)^{\beta_2} \left(\frac{\Delta t^n}{\Delta t^{n-1}}\right)^{-\alpha_2} \Delta t^n, \tag{13}$$

where ϵ is determined with $\epsilon = c\,TOL_t$, and $p \cdot \beta_1 = p \cdot \beta_2 = \alpha_2 = \frac{1}{4}$ with p being the order of the embedded method of the ESDIRK or ROW-scheme. c is included as a safety margin, a typical value is 0.9.

The controller needs to be started with the classic controller:

$$\Delta t^{n+1} = \left(\frac{\epsilon}{r_n}\right)^{\frac{1}{p}} \Delta t^n. \tag{14}$$

Step size rejections may be reduced by basing the test on the requested change ρ^n instead on the error estimate. Also, discontinuities in the step size change ratio $\frac{\Delta t^{n+1}}{\Delta t^n}$ are removed by applying a smooth limiter. Thus, the new step size is determined via $\Delta t^{n+1} = \widehat{\rho^n}\,\Delta t^n$, where ρ^n is given by

$$\rho^n = \left(\frac{\epsilon}{r^n}\right)^{\beta_1} \left(\frac{\epsilon}{r^{n-1}}\right)^{\beta_2} \left(\rho^{n-1}\right)^{-\alpha_2}, \tag{15}$$

and the smooth limiter gives $\widehat{\rho^n}$ with $\kappa = 2$:

$$\widehat{\rho^n} = 1 + \kappa \arctan\left(\frac{\rho^n - 1}{\kappa}\right). \tag{16}$$

3 NON-LINEAR SYSTEMS OF EQUATIONS

The implicit Runge-Kutta schemes lead to a nonlinear system of equations of the form

$$\mathbf{u} = \tilde{\mathbf{u}} + \alpha\,\Delta t\,\hat{\mathbf{f}}\left(\mathbf{u}\right), \tag{17}$$

where $\mathbf{u} \in \mathbb{R}$ is the unknown vector, α is a parameter, and $\tilde{\mathbf{u}}$ is a given vector. The function $\hat{\mathbf{f}}\left(\mathbf{u}\right)$ performs the temporal and spatial discretisation of the computational domain. This problem is solved by the Newton-Raphson method, which effectively solves the root problem

$$\mathbf{F}\left(\mathbf{u}\right) = \mathbf{0}. \tag{18}$$

An inexact Newton method is employed, thus the following procedure is followed repeatedly until the convergence criteria are satisfied:

$$\begin{aligned} \left|\left|\frac{\partial \mathbf{F}\left(\mathbf{u}\right)}{\partial\,\mathbf{u}}\Big|_k \Delta\mathbf{u} + \mathbf{F}\left(\mathbf{u}_k\right)\right|\right| &\leqslant \eta_k\,||\,\mathbf{F}\left(\mathbf{u}_k\right)|| \\ \mathbf{u}_{k+1} &= \mathbf{u}_k + \Delta\,\mathbf{u}, \qquad k = 0, 1, 2, 3, ..., \end{aligned} \tag{19}$$

The linear system of the Newton method is solved by a Krylov subspace solver such as GMRES. Eisenstat and Walker's method [11] is used to determine the cut-off criterion η_k of the GMRES method with the parameters

$$\eta_k{}^A = \gamma \frac{||\mathbf{F}(\mathbf{u}_k)||^2}{||\mathbf{F}(\mathbf{u}_{k-1})||^2}, \tag{20}$$

and

$$\eta_k{}^B = \begin{cases} \eta_{max}, & k = 0, \\ \min\left(\eta_{max},\, \eta_k{}^A\right), & k > 0, \gamma\, \eta_{k-1}{}^2 \leqslant 0.1 \\ \min\left(\eta_{max},\, \max\left(\eta_k{}^A, \gamma\, \eta_{k-1}{}^2\right)\right) & k > 0, \gamma\, \eta_{k-1}{}^2 > 0.1 \end{cases}, \tag{21}$$

wherein $\gamma = 0.9$. In order to avoid over solving of the final step of Newton method, the norm of the current nonlinear residual $||\mathbf{F}(\mathbf{u}_k)||$ is compared to the nonlinear residual norm at which the iterations would stop

$$\tau_t = \tau_a + \tau_r\, ||\mathbf{F}(\mathbf{u}_k)||, \tag{22}$$

for an absolute τ_a and a relative τ_r convergence criterion. η_k is bounded from below by a constant multiple of $\frac{\tau_t}{||\mathbf{F}(\mathbf{u}_k)||}$. The cut-off criterion η_k is determined with

$$\eta_n = \min\left(\eta_{max},\, \max\left(\eta_k{}^B,\, \frac{0.5\,\tau_t}{||\mathbf{F}(\mathbf{u}_k)||}\right)\right). \tag{23}$$

The matrix-vector products required by GMRES are estimated via a second order finite difference scheme

$$\frac{\partial\, \mathbf{F}(\mathbf{u})}{\partial\, \mathbf{u}}\mathbf{v} \approx \frac{\mathbf{F}(\mathbf{u} + \epsilon\, \mathbf{v}) - \mathbf{F}(\mathbf{u} - \epsilon\, \mathbf{v})}{2\, \epsilon}, \tag{24}$$

where the finite difference step ϵ is determined with

$$\epsilon = \frac{\sqrt{1 + ||\mathbf{u}||}}{||\mathbf{v}||} \sqrt[3]{\frac{\epsilon_{mach}}{2}}, \tag{25}$$

with ϵ_{mach} being the machine precision [12]. A first order approximation can also be used in order to decrease computational costs. However, preliminary computations showed that a second order approximation was necessary in order to increase the robustness of the method when applied to the Rosenbrock schemes.

An ILU preconditioner is used in order to decrease the condition number of the system matrix, and thus accelerating the convergence of GMRES.

4 RESULTS FOR A NON-LINEAR CONVECTION-DIFFUSION PROBLEM

This first test case consists of a generalised non-linear convection-diffusion equation:

$$u_t = \beta\, u^n \cdot \nabla u + \alpha \nabla \cdot (u^m\, \nabla u), \qquad x \in \Omega := (0,1) \times (0,1), \tag{26}$$

where $u(x, y, 0)$ is given by

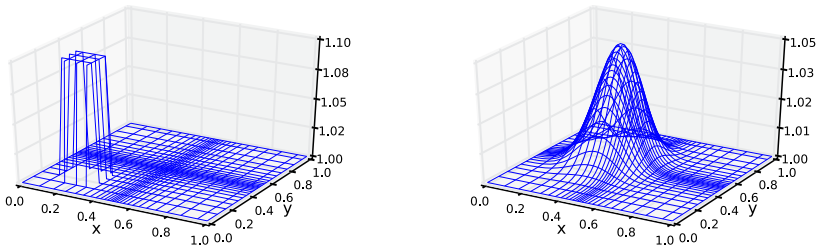
$$u(x, y, 0) = u_0(x, y). \tag{27}$$

The strength of the diffusion is determined by the parameter $\alpha \in \mathbb{R}$. The strength and the direction of the convection is determined with

$$\beta = \tilde{\beta} \begin{pmatrix} \sin(\gamma) \\ \cos(\gamma) \end{pmatrix}, \tag{28}$$

where $\tilde{\beta} \in \mathbb{R}$ is a user specified parameter, and γ determines the angle of the direction of the convection. The degree of non linearity is determined with the parameters m and n. The initial solution used for this test case is shown in Figure 1(a). The initial solution is one in the complete domain, except on the square $[0.1, 0.3] \times [0.1, 0.3]$, where the initial value is 1.1. The values for α, β and γ are set to $\alpha = 1$, $\beta = 200$ and $\gamma = 0.35\,\pi$. The reference solution at the end of the simulation is shown graphically in Figure 1(b) for $n = m = 1$.

A non-uniform mesh is used for the computations shown in this section (50×50). As shown in Figure 1, the mesh is refined close to $x = 0.5$ and $y = 0.5$ resulting in cells with a high aspect ratio. The maximum aspect ratio of the non-uniform mesh is 9.8. The condition number of $\mathbf{L}$ is relatively low for a uniform mesh. Hence, preconditioning is not necessary. Therefore, there is no obvious advantage of a constant system matrix $\mathbf{L}$ for a uniform mesh.



(a) Initial solution

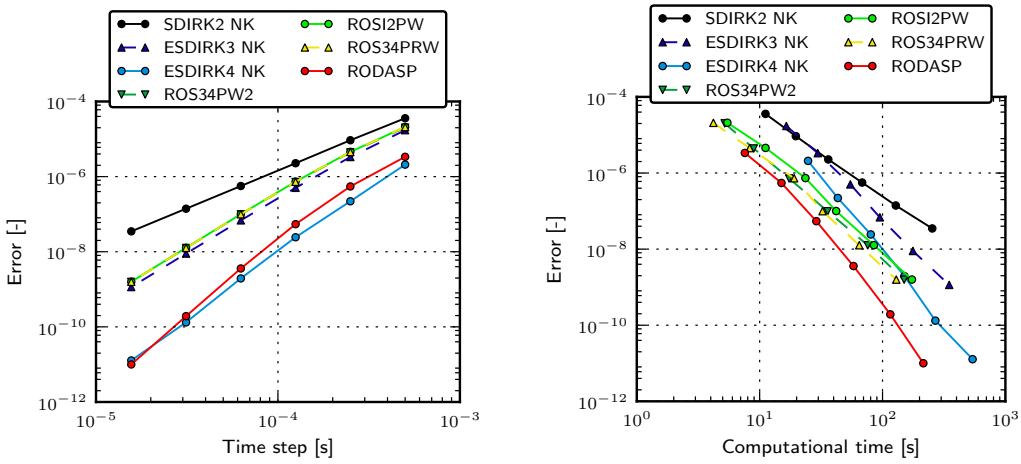
(b) Reference solution at time $t = 0.002$.

Figure 1: Initial solution and reference solution for a non-linear convection-diffusion simulation. The reference solution has been obtained with ESDIRK5 and $\Delta t = 10^{-7}$.

4.1 Effect of the Newton-Krylov method on accuracy and efficiency

The effect of the use of the Newton-Krylov method for the ESDIRK and Rosenbrock schemes is investigated. The results of simulations are shown in Figure 2. The ROW-schemes show a gain in efficiency compared to ESDIRK for the range of time step sizes. A small difference in accuracy is observed between the ESDIRK and ROW-schemes, where

the ESDIRK schemes show a slightly higher accuracy. RODASP has the greatest potential for use in a flow solver, since the computational time is reduced by approximately factor 2.5 compared to ESDIRK4.



(a) Accuracy **(b)** Computational work

Figure 2: Fixed time step study performed with the Newton-Krylov method for the non-linear convection-diffusion problem

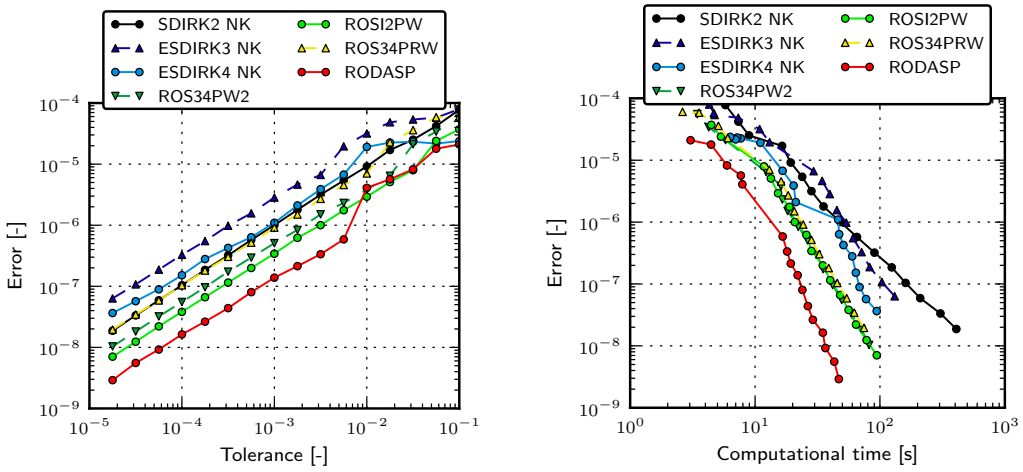
4.2 Effect of adaptive time step control on accuracy and efficiency

The effect of the use of the adaptive time step selection on accuracy and efficiency for the non-linear convection-diffusion case is shown in Figure 3. A difference in accuracy is observed between the different schemes for equal adaptive tolerance settings. Therefore it is necessary to perform a tolerance calibration in order to get the same accuracies for the different methods for a given tolerance [10].

Comparing the computational efficiency of ESDIRK and Rosenbrock shows a gain in efficiency for the Rosenbrock schemes. RODASP is the most computationally efficient scheme in comparison with the other time integration schemes for which the computational time reduced by a factor 3 to 4 compared to ESDIRK4.

5 RESULTS FOR A UNIFORM FLOW PAST A CIRCULAR CYLINDER

Following the previous non-linear convection-diffusion test case, the question remains how the ROW-scheme compares to the ESDIRK scheme in terms of computational efficiency and stability when applied to viscous flows. The second test case consists of a two-dimensional flow around a cylinder. The circular cylinder is held fixed in a uniform flow field, resulting in a vortex-street behind the cylinder. When the initial transient has disappeared, an unsteady periodic flow is present. This test case has been used in [13]



(a) Accuracy **(b)** Computational work

Figure 3: Comparison of efficiency and accuracy with adaptive time step control applied

and [1] to study the order of the ESDIRK schemes in comparison with BDF2.

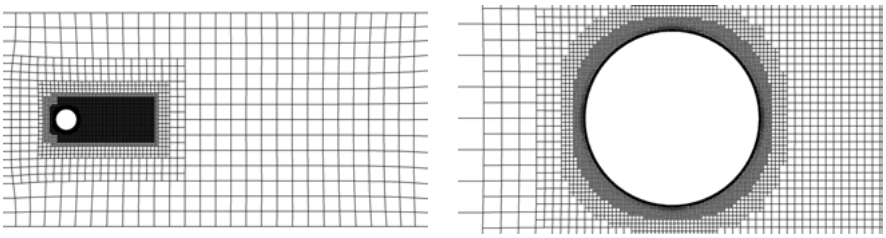
5.1 Description of the flow past a circular cylinder

The cylinder with diameter D is located on a fixed position in a uniform flow field with Mach number $M_\infty = 0.3$ and Reynolds number $Re_\infty = 1.0 \cdot 10^3$, simulating a laminar flow. The radius of the cylinder is used as the characteristic length to determine the Reynolds number.

The computational domain consists of $2.5D$ upstream of the centre of the cylinder, $4.5D$ above and below the cylinder centre, and $16.5D$ downstream of the centre of the cylinder. The mesh is refined in twelve steps to obtain a highly refined region close to the cylinder and in the wake downstream, resulting in a mesh with 10 608 cells. Close to the cylinder five extra layers of body conformal cells are generated resulting in an accurate representation of the boundary layer. The smallest cells which are located in the boundary layer, are of size $6.6 \cdot 10^{-5}\, D$. The maximum aspect ratio of the cells in the mesh is $6.3D$, and the minimum aspect ratio is $1.0D$. Refinement in the wake is performed, since the vortex street needs to be resolved accurately to obtain a good accuracy for the simulations. The generated mesh in shown in Figure 4.

5.2 Effect of the Newton-Krylov method on accuracy and efficiency

A fixed time step study has been performed for the ESDIRK and Rosenbrock time integration schemes. A non-linear multi grid solver [14] and Jacobian-free Newton-Krylov solver are used to solve the implicit stages of the ESDIRK scheme, and GMRES for the stages of the Rosenbrock scheme.

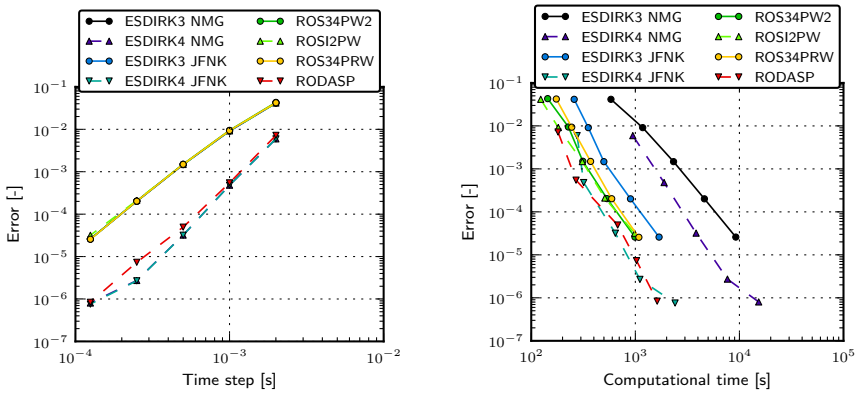


(a) Computational mesh **(b)** Computational mesh near the cylinder

Figure 4: Computational mesh used for the uniform flow around a circular cylinder case

The accuracy of the other computations performed with a Rosenbrock scheme lie close to the computations performed with an ESDIRK scheme. The order of the fourth order schemes reduces for small time steps, which is caused by the iterative error originating from the use of the Newton-Krylov and GMRES solvers.

A gain in computational efficiency is observed for the ROW-schemes in comparison with ESDIRK. The JFNK solver shows a significant increase in computational efficiency compared to the multi grid solver. The performance of RODASP is close to ESDIRK4.



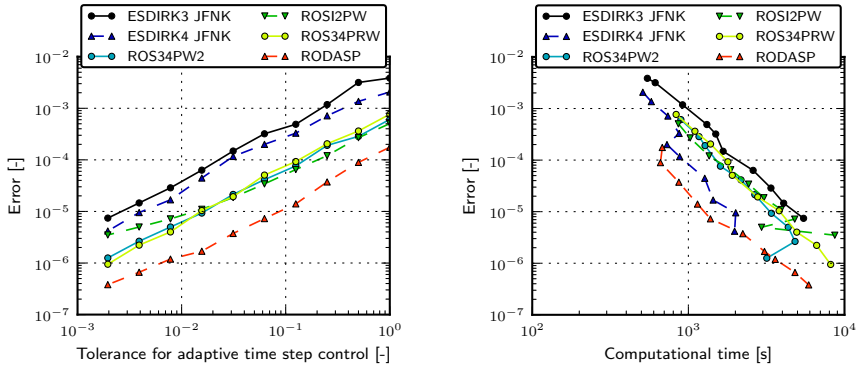
(a) Accuracy **(b)** Computational work

Figure 5: Computational work and accuracy for a fixed time step study

5.3 Effect of adaptive time step control on accuracy and computational stability for a uniform flow around a cylinder

Figure 6 shows the results of the numerical study comparing the accuracy and efficiency of ESDIRK and Rosenbrock when an adaptive time step control algorithm is employed. A large difference in accuracy for the same tolerance setting is observed when Rosenbrock and ESDIRK are compared. For the ROW-schemes, the accuracy of the solution is

more than one magnitude higher compared to ESDIRK3 and ESDIRK4. This difference in accuracy is comparable to the convection-diffusion case, indicating the possibility to perform a tolerance calibration and reuse the found coefficients for different problems. Also, a significant gain in efficiency is observed for the Rosenbrock schemes in comparison with ESDIRK.



(a) Accuracy **(b)** Computational work

Figure 6: Computational work and accuracy with adaptive time step selection

6 CONCLUSIONS

The computational efficiency and accuracy of ROW-schemes are compared with ESDIRK schemes for a non-linear convection-diffusion problem, and a laminar 2D flow around a cylinder. The numerical studies focused on the effects of using a fixed time or adaptive time step control algorithm on efficiency and accuracy of the simulations.

The main observation is that the ROW-schemes ROS34PRW and RODASP outperform the ESDIRK schemes in terms of computational efficiency. A difference in accuracy is observed when an adaptive time steps control method is used indicating that a tolerance calibration is necessary.

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